Connecting via Winsock to STN

Welcome to STN International! Enter x:X

LOGINID:SSPTAJMR1617

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

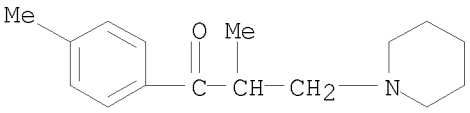
NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	3	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	4	MAR 31	CA/CAplus and CASREACT patent number format for U.S. applications updated
NEWS	5	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	6	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	7	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	8	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	9	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	10	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	11	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	12	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	13	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	14	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	15	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	16	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	17	JUN 25	CA/CAplus and USPAT databases updated with IPC reclassification data
NEWS	18	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS	19	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS	20	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS	21	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS	22	JUL 28	CA/CAplus patent coverage enhanced
NEWS	23	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS	24	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	25	JUL 28	STN Viewer performance improved
NEWS	26	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

```
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 18:45:04 ON 12 AUG 2008

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 18:45:17 ON 12 AUG 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   11 AUG 2008  HIGHEST RN 1040235-14-0
DICTIONARY FILE UPDATES:  11 AUG 2008  HIGHEST RN 1040235-14-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> "tolperisone"/cn
"TOLPERISONE" IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s "tolperisone"/cn
L1            1 "TOLPERISONE"/CN

=> d l1

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   728-88-1  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   1-Propanone, 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)-  (CA INDEX
```

NAME)
OTHER CA INDEX NAMES:
CN Propiophenone, 2,4'-dimethyl-3-piperidino- (7CI, 8CI)
OTHER NAMES:
CN (±)-Tolperisone
CN 2,4'-Dimethyl-3-piperidinopropiophenone
CN dl-Tolperisone
CN Mideton
CN Mydeton
CN Mydetone
CN NSC 107321
CN Tolperisone
DR 112537-33-4
MF C16 H23 N O
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DRUGU, EMBASE, IMSCOSEARCH, IMSDRUGNEWS, IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, MRCK*, PHAR, PROMT, PS, RTECS*, TOXCENTER, USAN, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

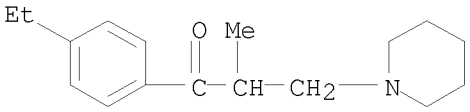
156 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
156 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> s "eperisone"/cn
L2 1 "EPERISONE"/CN

=> d l2

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 64840-90-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Propanone, 1-(4-ethylphenyl)-2-methyl-3-(1-piperidinyl)- (CA INDEX NAME)
OTHER NAMES:
CN (±)-Eperisone
CN 4'-Ethyl-2-methyl-3-piperidinopropiophenone
CN Eperisone
DR 124308-54-9
MF C17 H25 N O
CI COM
LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CIN, DDFU, DRUGU, EMBASE, IMSPATENTS,

IMSPRODUCT, IMSRESEARCH, MRCK*, PHAR, PROMT, PROUSDDR, PS, RTECS*,
SYNTHLINE, TOXCENTER, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: WHO



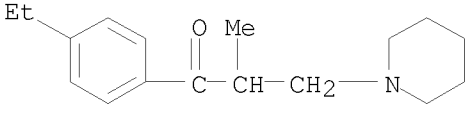
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

94 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
94 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s l1 or l2
L3 2 L1 OR L2

=> d l3

L3 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN
RN 64840-90-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Propanone, 1-(4-ethylphenyl)-2-methyl-3-(1-piperidinyl)- (CA INDEX NAME)
OTHER NAMES:
CN (±)-Eperisone
CN 4'-Ethyl-2-methyl-3-piperidinopropiophenone
CN Eperisone
DR 124308-54-9
MF C17 H25 N O
CI COM
LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CIN, DDFU, DRUGU, EMBASE, IMSPATENTS, IMSPRODUCT, IMSRESEARCH, MRCK*, PHAR, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: WHO



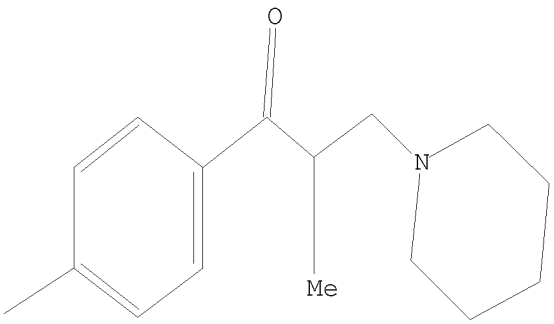
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

94 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
94 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>
Uploading C:\Program Files\STNEXP\Queries\10551510_2.str

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> sea sss sam l4
SAMPLE SEARCH INITIATED 18:53:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 182 TO ITERATE

100.0% PROCESSED 182 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2831 TO 4449
PROJECTED ANSWERS: 7 TO 298

L5 7 SEA SSS SAM L4

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 22.74 22.95

FILE 'CAPLUS' ENTERED AT 18:53:45 ON 12 AUG 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907 - 12 Aug 2008 VOL 149 ISS 7
FILE LAST UPDATED: 11 Aug 2008 (20080811/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> sea abb=ON Plu=on l4
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 18:54:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 182 TO ITERATE

100.0% PROCESSED 182 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2831 TO 4449
PROJECTED ANSWERS: 7 TO 298

L6 7 SEA SSS SAM L4

L7 6 L6

=> d ibib ab histr l7
'HISTR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels

```
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
information will be displayed in the same order as the format
specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):d ibib ab histr 1-7
'D' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS
```

```
IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
information will be displayed in the same order as the format
specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):d ibib ab hitstr 1-7
'D' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
```

```
              e.g., D SCAN or DISPLAY SCAN)
STD ---------- BIB, CLASS

IABS --------- ABS, indented with text labels
IALL --------- ALL, indented with text labels
IBIB --------- BIB, indented with text labels
IMAX --------- MAX, indented with text labels
ISTD --------- STD, indented with text labels

OBIB --------- AN, plus Bibliographic Data (original)
OIBIB -------- OBIB, indented with text labels

SBIB --------- BIB, no citations
SIBIB -------- IBIB, no citations

HIT ---------- Fields containing hit terms
HITIND ------- IC, ICA, ICI, NCL, CC and index field (ST and IT)
               containing hit terms
HITRN -------- HIT RN and its text modification
HITSTR ------- HIT RN, its text modification, its CA index name, and
               its structure diagram
HITSEQ ------- HIT RN, its text modification, its CA index name, its
               structure diagram, plus NTE and SEQ fields
FHITSTR ------ First HIT RN, its text modification, its CA index name, and
               its structure diagram
FHITSEQ ------ First HIT RN, its text modification, its CA index name, its
               structure diagram, plus NTE and SEQ fields
KWIC --------- Hit term plus 20 words on either side
OCC ---------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
information will be displayed in the same order as the format
specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):file caplus
'FILE' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'
'CAPLUS' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ---------- GI and AB
ALL ---------- BIB, AB, IND, RE
APPS --------- AI, PRAI
BIB ---------- AN, plus Bibliographic Data and PI table (default)
CAN ---------- List of CA abstract numbers without answer numbers
CBIB --------- AN, plus Compressed Bibliographic Data
CLASS -------- IPC, NCL, ECLA, FTERM
DALL --------- ALL, delimited (end of each field identified)
DMAX --------- MAX, delimited for post-processing
FAM ---------- AN, PI and PRAI in table, plus Patent Family data
FBIB --------- AN, BIB, plus Patent FAM
IND ---------- Indexing data
IPC ---------- International Patent Classifications
MAX ---------- ALL, plus Patent FAM, RE
PATS --------- PI, SO
```

```
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
information will be displayed in the same order as the format
specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):bib

L7   ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2001:372573  CAPLUS
DN   135:152695
TI   Synthesis, resolution and absolute configuration of a tolperisone
     metabolite
AU   Balint, J.; Markovits, I.; Egri, G.; Tuza, Z.; Parkanyi, L.; Fogassy, E.
CS   Department of Organic Chemical Technology, Budapest University of
     Technology and Economics, Budapest, H-1521, Hung.
SO   Tetrahedron: Asymmetry (2001), 12(5), 719-724
     CODEN: TASYE3; ISSN: 0957-4166
PB   Elsevier Science Ltd.
DT   Journal
LA   English
OS   CASREACT 135:152695
RE.CNT  15    THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
```

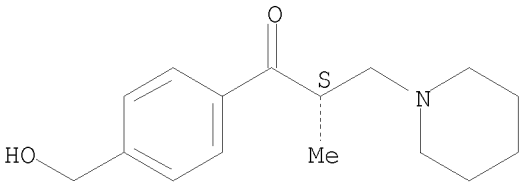
=> d ibib ab hitstr 1-6

L7 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:372573 CAPLUS
DOCUMENT NUMBER: 135:152695
TITLE: Synthesis, resolution and absolute configuration of a tolperisone metabolite
AUTHOR(S): Balint, J.; Markovits, I.; Egri, G.; Tuza, Z.; Parkanyi, L.; Fogassy, E.
CORPORATE SOURCE: Department of Organic Chemical Technology, Budapest University of Technology and Economics, Budapest, H-1521, Hung.
SOURCE: Tetrahedron: Asymmetry (2001), 12(5), 719-724
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:152695
AB 1-(4'-Hydroxymethyl-phenyl)-2-methyl-3-(piperidine-1-yl)-propane-1-one (M2, I), a metabolite of tolperisone, was synthesized as its hydrochloride salt in a solvent-free Mannich reaction. The optical resolution of I·HCl was carried out by diastereoisomeric salt formation and separation, for which three resolving agents (2R,3R)-O,O'-dibenzoyltartaric acid, (2R,3R)-O,O'-di-p-toluoyltartaric acid and (R)-2-hydroxy-4-(2-methoxyphenyl)-5,5-dimethyl-1,3,2-dioxaphosphorinane-2-oxide (anicyphos) were found. The absolute configuration of M2 was determined by the single-crystal X-ray diffraction method.
IT 352233-21-7P
RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(synthesis, resolution and absolute configuration of a tolperisone metabolite)
RN 352233-21-7 CAPLUS
CN Butanedioic acid, 2,3-bis(phenylmethoxy)-, (2R,3R)-(2S)-compd. with 1-[4-(hydroxymethyl)phenyl]-2-methyl-3-(1-piperidinyl)-1-propanone (1:1) (CA INDEX NAME)

CM 1

CRN 352233-17-1
CMF C16 H23 N O2

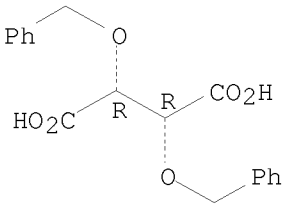
Absolute stereochemistry. Rotation (+).



CM 2

CRN 138794-81-7
CMF C18 H18 O6

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:566027 CAPLUS
DOCUMENT NUMBER: 131:184942
TITLE: Preparation of 3-(5-isoxazolyl)- or 3-phenylpropylamine derivatives as central muscle relaxants
INVENTOR(S): Matsui, Takeaki; Tanaka, Yuichiro; Inoue, Masaki; Etoh, Shugo; Noda, Masatoshi; Yabuki, Tetsuaki; Toga, Tetsuo; Amagishi, Hiroaki; Hayakawa, Maki; Tanaka, Chikage; Matsumura, Yumi
PATENT ASSIGNEE(S): Maruho Kabushikikaisha, Japan
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

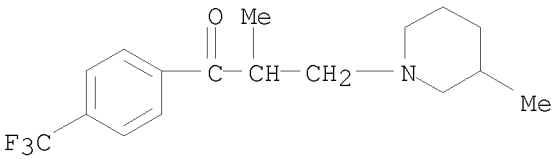
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9943656	A1	19990902	WO 1999-JP759	19990219
W: CN, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			JP 1998-43998 A	19980225
OTHER SOURCE(S):	MARPAT 131:184942			

AB Propylamine derivs. represented by formula ACH(O2CNHR5)CR1R2CH2NR3R4 and salts thereof (wherein A is substituted aryl or optionally substituted heteroaryl; R1 and R2 are the same or different lower alkyls, or one of R1 and R2 is hydrogen and the other is lower alkyl, lower alkoxy, aryl, aralkyl, or lower alkoxy- or lower alkylthio-substituted lower alkyl; one of R3 and R4 is hydrogen or lower alkyl and the other is lower cycloalkyl, or R3 or R4 are the same or different lower alkyls or are bonded to each other to form a ring which contains one or more nitrogen or oxygen atoms and is optionally substituted by lower alkyl, lower alkanoyl, or aralkyl; and R5 is hydrogen, lower alkyl, or aryl) are prepared These compds. are useful as central muscle relaxants or for the treatment of urination disorders. Thus, (1R,2R)-5-[1-hydroxy-2-(1-pyrrolidinylmethyl)butyl]-3-phenylisoxazole was condensed with Ph chlorocarbonate in pyridine/CH2Cl2 at room temperature for 2 h and the amidated with NH3 in 2-propanol at room temperature for 4 h to give, after salt formation with oxalic acid, (1R,2R)-5-[1-(carbamoyloxy)-2-(1-pyrrolidinylmethyl)butyl]-3-phenylisoxazole [I.(CO2H)2]. I.(CO2H)2 at 4.0 mg/kg p.o relaxed 84.7% decerebrate rigidity in rats.
IT 240124-69-0
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

RN 240124-69-0 CAPLUS

CN 1-Propanone, 2-methyl-3-(3-methyl-1-piperidinyl)-1-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:194509 CAPLUS

DOCUMENT NUMBER: 126:242800

ORIGINAL REFERENCE NO.: 126:46885a,46888a

TITLE: Preparation and investigation of products containing tolperisone-HCl and CDs

AUTHOR(S): Antal, L.; Dombi, Gy.; Novak, Cs.; Kata, M.

CORPORATE SOURCE: Department of Pharmaceutical Technology, Albert Szent-Gyorgyi Medical University, Szeged, H-6720, Hung.

SOURCE: Proceedings of the International Symposium on Cyclodextrins, 8th, Budapest, Mar. 31-Apr. 2, 1996 (1996), 301-303. Editor(s): Szejtli, J.; Szente, L. Kluwer: Dordrecht, Neth.
CODEN: 64CDAL

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The aim of the paper was to study the conditions of complex formation of tolperisone-HCl with different cyclodextrins (CD) such as α-CD, β-CD, γ-CD, dimethyl-β-CD and randomly methylated β-CD by using various preparation techniques and investigation methods.

IT 188483-72-9P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of drug-cyclodextrin complexes)

RN 188483-72-9 CAPLUS

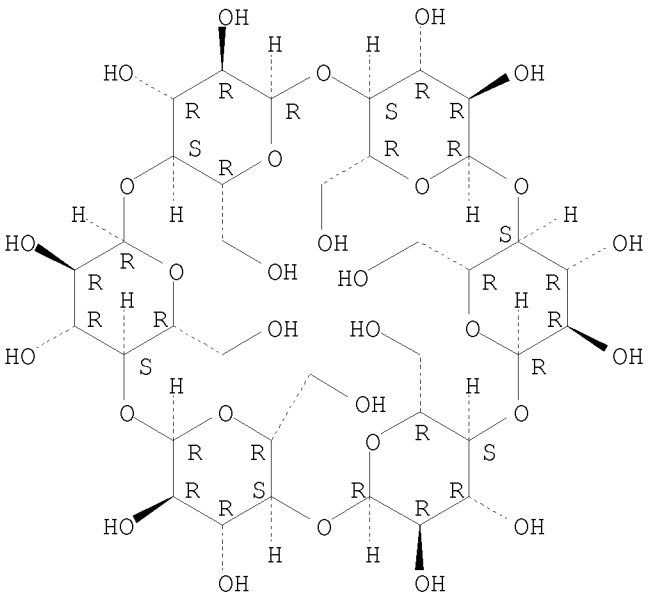
CN α-Cyclodextrin, compd. with 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)-1-propanone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 10016-20-3

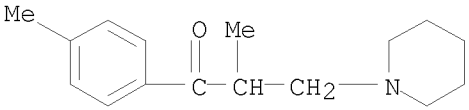
CMF C36 H60 O30

Absolute stereochemistry.



CM 2

CRN 728-88-1
CMF C16 H23 N O



L7 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:594968 CAPLUS
DOCUMENT NUMBER: 121:194968
ORIGINAL REFERENCE NO.: 121:35111a,35114a
TITLE: A new quantum chemical approach in QSAR-analysis: parametrization of conformational energies into molecular descriptors JMn (steric) and JSn (electronic)
AUTHOR(S): Joshi, R. K.; Meister, T.; Scapozza, L.; Ha, T.-K.
CORPORATE SOURCE: Department Pharmacy, Swiss Federal Institute Technology, Zurich, Switz.
SOURCE: Arzneimittel-Forschung (1994), 44(6), 779-90
CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE: Journal
LANGUAGE: English

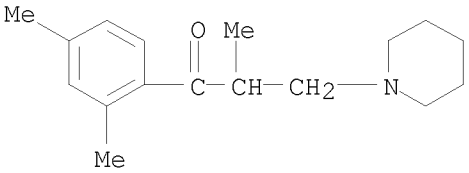
AB Two new types of structure-related mol. descriptors JMn and JSn, have been developed using conformational energies from quantum chemical calcns. For this purpose propipocaine (CAS 3670-68-6) was chosen as a model and 42 analogs were studied. The quantum chemical calcns. were performed applying AM1 and PCILO approximation methods. Appropriate math. models were designed to calculate steric parameter log JM1 and electronic parameters JS1 to JS6. The values obtained for these parameters were used in multiple linear regression anal. for the evaluation of the structure-activity relationship. Furthermore, a comparison between electronic parameters JSn

and σ (Hammett) was made. The results show that these parameters can be used successfully in predicting the biol. activity of compds. in this model. Although, JS5 values are comparable to σ-Hammett, the electronic parameter JS2 gives a better correlation in QSAR-anal. involving two parameters JS2 and log JM1.

IT 158176-65-9
RL: BIOL (Biological study)
(anesthetic QSAR anal. of, parametrization of conformational energies into steric and electronic mol. descriptors in)

RN 158176-65-9 CAPLUS

CN 1-Propanone, 1-(2,4-dimethylphenyl)-2-methyl-3-(1-piperidinyl)- (CA INDEX NAME)



L7 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:509128 CAPLUS

DOCUMENT NUMBER: 89:109128

ORIGINAL REFERENCE NO.: 89:16801a,16804a

TITLE: Tolperisone optical isomers and their salts

INVENTOR(S): Furuta, Yasuhiko; Nakamura, Keita; Tashiro, Yasuhisa; Aoki, Shigeru; Nagashima, Takashi

PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53040779	A	19780413	JP 1976-113385	19760921

PRIORITY APPLN. INFO.: JP 1976-113385 A 19760921

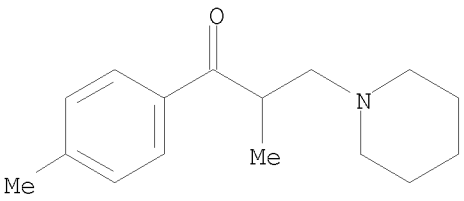
AB Optical resolution of dl-I with N-acetyl-D-phenylglycine (D-II) or L-II in Me2CO or MeCOEt gave d- or l-I, resp. D-I had higher central muscle-relaxant activity than l-I, whereas l-I had higher bronchodilatory and peripheral vasodilatory activities than d-I. Thus, 0.25 mol each of dl-I and D-II in Me2CO was seeded and kept cold overnight to give 0.122 mol d-I-D-II salt, which was converted to d-I.HCl. Similarly prepared were l-I-L-II salt and l-I.HCl.

IT 67499-62-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and pharmacol. activity of)

RN 67499-62-1 CAPLUS

CN 1-Propanone, 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)-, hydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



● HCl

L7 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:104761 CAPLUS
DOCUMENT NUMBER: 68:104761
ORIGINAL REFERENCE NO.: 68:20206h,20207a
TITLE: (α-Alkylideneacl)phenylalkanoic acids
INVENTOR(S): Schultz, Everett M.; Sprague, James M.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3352903		19671114	US 1963-253042	19630122

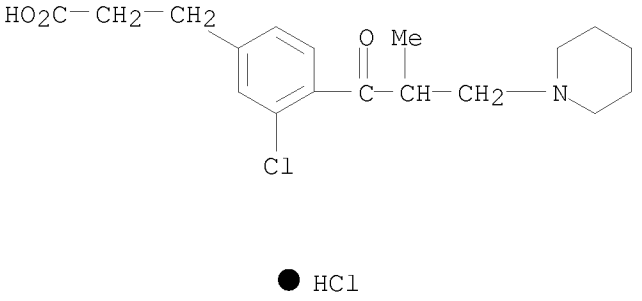
AB The title compds. were prepared by converting the corresponding saturated acyl compds. which lack the α-methylene group to the salt of a Mannich base by reaction with a salt of a secondary amine in the presence of H2CO and treatment of the Mannich salt with a base. EtCOCl (11.1 g.) was added dropwise to a stirred mixture of 18.5 g. m-ClC6H4(CH2)2CO2H, 40 g. chloride, and 140 g. CS2, the mixture refluxed 3.5 hrs. to give 3.5 g. 3,4-R1(RCO)C6H3(CH2)2CO2H (I, R = Et, R1 = Cl) (II), m. 67-70° (cyclohexane-C6H6). A mixture of 8.5 g. II, 1.5 g. paraformaldehyde, 4.9 g. piperidine-HCl salt and 1 ml. ethanolic HCl was heated 1.5 hrs. on the steam bath, the resulting syrup dissolved in 70 ml. hot iso-PrOH, and cooled to give 6.3 g. 3-[3-chloro-4-[2-(1-piperidylmethyl)propionyl]phenyl]propionic acid (III).HCl, m. 143-6°. A solution of 6.3 g. III, HCl salt in 80 ml. saturated NaHCO3 solution was kept 1 hr. at room temperature, and the solution acidified to give 1.3 g. 3,4-R2[RC(:CHR1)CO]C6H3(CH2)2CO2H (IV, R = Me, R1 = H, R2 = Cl), m. 78.5-80° (cyclohexane-C6H6). Other I prepared were (R and R1 given): Pr, H (m. 104-5° in 46% yield); iso-Pr(CH2)2, Cl; Pr, Br; hexyl, Cl; Pr, Me; (CH2)2CO2H, Me; (CH2)2CF3, Me; (CH2)3Cl, Me; (CH2)2SPh, Me; morpholinopropyl, Me; cyclohexylmethyl, Cl; Pr, OMe. Other IV prepared were (R, R1, R2 given): H, Me, H (m. 94-6° in 43% yield); H, iso-PrCH2CH, Cl; H, Me, Br; H, hexyl, Cl; H, Me, Me; H, CO2H, Me; H, CF3, Me; H, CH2SPh, Me; H, morpholinomethyl, Me; H, cyclohexyl, Cl; p-tolyl, H, Cl; Ph, H, Cl; H, Me, OMe. The corresponding butyric acids may be similarly prepared A solution of 3-[3-bromo-4-(2-methylenebutyryl)phenyl]propionic acid in iso-PrOH was reduced over Pd-C at 35 psig. to give 3-[3-bromo-4-(2-methylbutyryl)phenyl]propionic acid (V). A solution of V in HOAc was treated dropwise with stirring with an equivalent amount of Br in HOAc (the reaction was initiated with 2 drops 48% HBr), the mixture added to H2O containing a little

NaHSO3 and the 3-[3-bromo-4-(2-bromo-2-methylbutyryl)phenyl]propionic acid (VI) collected. A mixture of VI, LiBr, and HCONMe2 was heated 4 hrs. at 80-90°, the mixture poured into H2O to give IV (R = Et, R1 = H, R2 = Br). These compds. possess diuretic, natriuretic, and chloriuretic properties, and are, therefore useful in the treatments of ailments associated with electrolyte retention.

IT 19445-68-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19445-68-2 CAPLUS

CN Hydrocinnamic acid, 3-chloro-4-(2-methyl-3-piperidinopropionyl)-, hydrochloride (8CI) (CA INDEX NAME)



=>

=> l6 and pain
L6 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s l6 and pain
6 L6
60992 PAIN
L8 0 L6 AND PAIN

=> s l6 and spasticity
6 L6
1082 SPASTICITY
L9 0 L6 AND SPASTICITY

=> s l6 and spasm
6 L6
5286 SPASM
L10 0 L6 AND SPASM

=> s l6 and NMDA
6 L6
29908 NMDA
L11 0 L6 AND NMDA

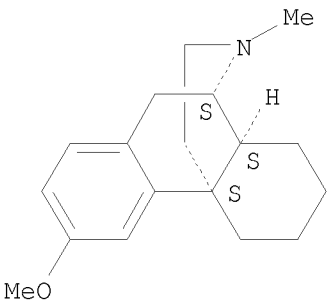
=> s (l1 or l2) AND NMDA
156 L1
94 L2
29908 NMDA
L12 1 (L1 OR L2) AND NMDA

```
=> d l12 ibib

L12  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        1997:799525  CAPLUS
DOCUMENT NUMBER:         128:110783
ORIGINAL REFERENCE NO.:  128:21597a,21600a
TITLE:                   Comparative characterization of the centrally acting
                         muscle relaxant RGH-5002 and tolperisone and of
                         lidocaine based on their effects on rat spinal cord in
                         vitro
AUTHOR(S):               Farkas, S.; Kocsis, P.; Bielik, N.
CORPORATE SOURCE:        Pharmacological Research Centre, Gedeon Richter Ltd.,
                         Budapest, H-1475, Hung.
SOURCE:                  Neurobiology (Budapest) (1997), 5(1), 57-58
                         CODEN: NROBEZ; ISSN: 1216-8068
PUBLISHER:               Akademiai Kiado
DOCUMENT TYPE:           Journal
LANGUAGE:                English


=> d l12 abs ibib

L12  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
AB   A direct effect of RGH-5002, the centrally acting muscle relaxant, on the
     spinal cord was investigated in vitro.  For comparison, the effects of
     tolperisone and the local anesthetic lidocaine were also studied.  The
     ventral root potential evoked by supramaximal dorsal root stimulation was
     recorded using suction electrodes for both stimulation and recording from
     hemisected spinal cords excised from 6 day-old rats.  From the fact that
     all three drugs strongly diminished a prolonged depolarization of the
     ventral root including its very early part preceding monosynaptic reflex
     and that they did not possess glutamate (AMPA and NMDA)
     antagonist effect, it may be concluded that these drugs depressed the
     transmitter release from presynaptic terminals.  The quant. profile of the
     effects of the three drugs on the different components of the reflux
     suggest that the mechanism of action of lidocaine is somewhat different,
     whereas tolperisone and RGH-5002 are more similar to each other.
ACCESSION NUMBER:        1997:799525  CAPLUS
DOCUMENT NUMBER:         128:110783
ORIGINAL REFERENCE NO.:  128:21597a,21600a
TITLE:                   Comparative characterization of the centrally acting
                         muscle relaxant RGH-5002 and tolperisone and of
                         lidocaine based on their effects on rat spinal cord in
                         vitro
AUTHOR(S):               Farkas, S.; Kocsis, P.; Bielik, N.
CORPORATE SOURCE:        Pharmacological Research Centre, Gedeon Richter Ltd.,
                         Budapest, H-1475, Hung.
SOURCE:                  Neurobiology (Budapest) (1997), 5(1), 57-58
                         CODEN: NROBEZ; ISSN: 1216-8068
PUBLISHER:               Akademiai Kiado
DOCUMENT TYPE:           Journal
LANGUAGE:                English


=> s (l1 or l2) AND pain
           156 L1
            94 L2
         60992 PAIN
L13         18 (L1 OR L2) AND PAIN
```

```
=> s (l1 or l2) SAME pain
MISSING OPERATOR L2) SAME
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s (l1 or l2) near pain
MISSING OPERATOR L2) NEAR
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s (l1 or l2) with pain
MISSING OPERATOR L2) WITH
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s (l1 or l2) w pain
MISSING OPERATOR L2) W PAIN
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s (l1 or l2)abj pain
MISSING OPERATOR L2)ABJ
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s (l1 or l2) abj pain
MISSING OPERATOR L2) ABJ
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                  57.95      81.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                  -5.60      -5.60

FILE 'REGISTRY' ENTERED AT 19:03:12 ON 12 AUG 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   11 AUG 2008  HIGHEST RN 1040235-14-0
DICTIONARY FILE UPDATES:  11 AUG 2008  HIGHEST RN 1040235-14-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:
```

http://www.cas.org/support/stngen/stndoc/properties.html

```
=> s "dextromethophan"/cn
L14          0 "DEXTROMETHOPHAN"/CN

=> s "dextromethorphan"/cn
L15          1 "DEXTROMETHORPHAN"/CN

=> d l15

L15  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   125-71-3  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Morphinan, 3-methoxy-17-methyl-, (9α,13α,14α)-  (CA
     INDEX NAME)
OTHER CA INDEX NAMES:
CN   9α,13α,14α-Morphinan, 3-methoxy-17-methyl- (8CI)
OTHER NAMES:
CN   (+)-3-Methoxy-17-methylmorphinan
CN   Ba 2666
CN   d-Methorphan
CN   DEX
CN   Dextromethorphan
CN   Nodex
FS   STEREOSEARCH
DR   18046-32-7, 32062-10-5
MF   C18 H25 N O
CI   COM
LC   STN Files:   ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS,
       BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMLIST, CIN,
       CSCHEM, DDFU, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH,
       IPA, MEDLINE, PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS*, SCISEARCH,
       SPECINFO, TOXCENTER, USAN, USPAT2, USPATFULL, USPATOLD, VETU
         (*File contains numerically searchable property data)
     Other Sources:   EINECS**, WHO
         (**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

            2064 REFERENCES IN FILE CA (1907 TO DATE)
              60 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
            2071 REFERENCES IN FILE CAPLUS (1907 TO DATE)
```

4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      12.76      94.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -5.60

FILE 'CAPLUS' ENTERED AT 19:03:55 ON 12 AUG 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 12 Aug 2008  VOL 149 ISS 7
FILE LAST UPDATED: 11 Aug 2008  (20080811/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s (l1 or l2) and l15
           156 L1
            94 L2
          2071 L15
L16          7 (L1 OR L2) AND L15

=> d l16 abs ibib 1-7

L16  ANSWER 1 OF 7  CAPLUS  COPYRIGHT 2008 ACS on STN
AB   Disclosed herein is are methods to treat neuropsychiatric diseases
     including psychosis.  Treatment is carried out by administering a
     therapeutically effective amount of N-desmethylclozapine to a patient
     suffering from a neuropsychiatric disease.
ACCESSION NUMBER:        2008:10517  CAPLUS
DOCUMENT NUMBER:         148:93259
TITLE:                   Use of n-desmethylclozapine to treat psychosis
INVENTOR(S):             Weiner, David; Van Kammen, Daniel P.; Corritori,
                         Suzana
PATENT ASSIGNEE(S):      Acadia Pharmaceuticals Inc., USA
SOURCE:                  PCT Int. Appl., 88pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
```

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008002602	A1	20080103	WO 2007-US14897	20070626

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2006-817010P P 20060627
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AB Cytochromes P 450 3A4, 2D6, and 2C9 metabolize a large fraction of drugs. Knowing where these enzymes will preferentially oxidize a mol., the regioselectivity, allows medicinal chemists to plan how best to block its metabolism The authors present QSAR-based regioselectivity models for these enzymes calibrated against compiled literature data of drugs and drug-like compds. These models are purely empirical and use only the structures of the substrates, in contrast to those models that simulate a specific mechanism like hydrogen radical abstraction, and/or use explicit models of active sites. The authors most predictive models use three substructure descriptors and two phys. property descriptors. Descriptor importance from the random forest QSAR method show that other factors than the immediate chemical environment and the accessibility of the hydrogen affect regioselectivity in all three isoforms. The cross-validated predictions of the models are compared to predictions from the authors earlier mechanistic model (Singh et al. J. Med. Chemical 2003, 46, 1330-1336) and predictions from MetaSite (Cruciani et al. J. Med. Chemical 2005, 48, 6970-6979).
ACCESSION NUMBER: 2007:655403 CAPLUS
DOCUMENT NUMBER: 147:226154
TITLE: Empirical Regioselectivity Models for Human Cytochromes P450 3A4, 2D6, and 2C9
AUTHOR(S): Sheridan, Robert P.; Korzekwa, Kenneth R.; Torres, Rhonda A.; Walker, Matthew J.
CORPORATE SOURCE: Molecular Systems Department, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(14), 3173-3184
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AB A rapid, selective and robust direct-injection LC/hybrid tandem MS method has been developed for simultaneous screening of more than 250 basic drugs

in the supernatant of enzyme hydrolyzed equine urine. Analytes, trapped using a short HLB extraction column, are refocused and separated on a Sunfire C18 anal. column using a controlled differential gradient generated by proportional dilution of the first column's eluent with water. Independent data acquisition (IDA) was configured to trigger a sensitive enhanced product ion (EPI) scan when a multiple reaction monitoring (MRM) survey scan signal exceeded the defined criteria. The decision on whether or not to report a sample as a pos. result was based upon both the presence of a MRM response within the correct retention time range and a qual. match between the EPI spectrum obtained and the corresponding reference standard Ninety seven percent of the drugs targeted by this method met our detection criteria when spiked into urine at 100 ng/mL; 199 were found at 10 ng/mL, 83 at 1 ng/mL and 4 at 0.1 ng/mL.

ACCESSION NUMBER: 2006:452736 CAPLUS
DOCUMENT NUMBER: 145:97622
TITLE: Screening for basic drugs in equine urine using direct-injection differential-gradient LC-LC coupled to hybrid tandem MS/MS
AUTHOR(S): Stanley, Shawn M. R.; Foo, Hsiao Ching
CORPORATE SOURCE: Singapore Race Course, The Singapore Turf Club Laboratory, Singapore, 738078, Singapore
SOURCE: Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2006), 836(1-2), 1-14
CODEN: JCBAAI; ISSN: 1570-0232
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

AB Disclosed herein is a method to treat neuropsychiatric diseases including psychosis, affective disorders, dementia, neuropathic pain, and glaucoma. Treatment is carried out by administering a therapeutically effective amount of N-desmethylclozapine to a patient suffering from a neuropsychiatric disease.

ACCESSION NUMBER: 2005:1200866 CAPLUS
DOCUMENT NUMBER: 143:452893
TITLE: Use of N-desmethylclozapine to treat human neuropsychiatric disease
INVENTOR(S): Weiner, David M.; Brann, Mark R.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 913,117.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050250767	A1	20051110	US 2005-98892	20050404
US 20040224942	A1	20041111	US 2004-761787	20040121
US 20050085463	A1	20050421	US 2004-913117	20040805
AU 2005271513	A2	20060216	AU 2005-271513	20050804
AU 2005271513	A1	20060216		
CA 2576153	A1	20060216	CA 2005-2576153	20050804

WO 2006017614	A1	20060216	WO 2005-US27645		20050804
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
EP 1778244	A1	20070502	EP 2005-802835		20050804
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR					
CN 101094674	A	20071226	CN 2005-80033997		20050804
JP 2008509147	T	20080327	JP 2007-524968		20050804
US 20060194831	A1	20060831	US 2006-416565		20060503
US 20060199807	A1	20060907	US 2006-417069		20060503
US 20070275957	A1	20071129	US 2007-671405		20070205
PRIORITY APPLN. INFO.:			US 2003-442690P	P	20030123
			US 2004-761787	A2	20040121
			US 2004-913117	A2	20040805
			US 2004-617553P	P	20041008
			US 2005-98892	A	20050404
			WO 2005-US27645	W	20050804

L16 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

AB Disclosed herein is a method to treat neuropsychiatric diseases including psychosis, affective disorders, dementia, neuropathic pain, and glaucoma. Treatment is carried out by administering a therapeutically effective amount of N-desmethylclozapine to a patient suffering from a neuropsychiatric disease.

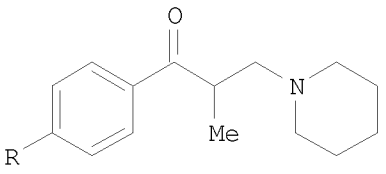
ACCESSION NUMBER: 2005:349001 CAPLUS
DOCUMENT NUMBER: 142:386016
TITLE: Use of N-desmethylclozapine to treat human neuropsychiatric disease
INVENTOR(S): Weiner, David M.; Brann, Mark R.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S Ser. No. 761,787.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050085463	A1	20050421	US 2004-913117	20040805
US 20040224942	A1	20041111	US 2004-761787	20040121
US 20050250767	A1	20051110	US 2005-98892	20050404
AU 2005271513	A2	20060216	AU 2005-271513	20050804
AU 2005271513	A1	20060216		
CA 2576153	A1	20060216	CA 2005-2576153	20050804
WO 2006017614	A1	20060216	WO 2005-US27645	20050804
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,				

NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM

EP 1778244	A1	20070502	EP 2005-802835	20050804
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 101094674	A	20071226	CN 2005-80033997	20050804
JP 2008509147	T	20080327	JP 2007-524968	20050804
US 20060194831	A1	20060831	US 2006-416565	20060503
US 20060199807	A1	20060907	US 2006-417069	20060503
US 20070275957	A1	20071129	US 2007-671405	20070205
IN 2007KN00526	A	20070706	IN 2007-KN526	20070213
PRIORITY APPLN. INFO.:			US 2003-442690P P	20030123
			US 2004-761787 A2	20040121
			US 2004-913117 A2	20040805
			US 2004-617553P P	20041008
			US 2005-98892 A	20050404
			WO 2005-US27645 W	20050804

L16 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
GI



I

AB The present invention relates to a pharmaceutical combination for the treatment of spasticity and/or pain characterized by that the combination contains as active ingredient 70-95% weight/weight compound of formula (I), wherein R represents a Me or Et group, and 5-30 % weight/weight dextromethorphan
(chemical name: (+/-)-3-methoxy-17-methylmorphinan).

ACCESSION NUMBER: 2004:872682 CAPLUS
DOCUMENT NUMBER: 141:370535
TITLE: Pharmaceutical combination for the treatment of spasticity and/or pain
INVENTOR(S): Tihanyi, Karoly; Kocsis, Pal; Nemeth, Gyoergy; Tarnawa, Istvan; Dalmadi, Balazs
PATENT ASSIGNEE(S): Richter Gedeon Vegyeszeti Gyar Rt., Hung.
SOURCE: PCT Int. Appl., 16 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089352	A2	20041021	WO 2004-HU32	20040407
WO 2004089352	A3	20041216		

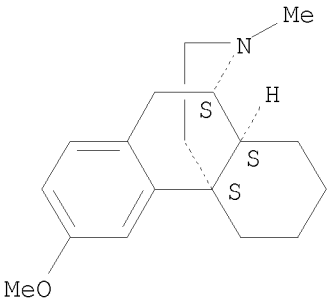
```
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
     HU 2003000929        A2    20050228    HU 2003-929           20030409
     HU 2003000929        A3    20050628
     EP 1610785           A2    20060104    EP 2004-726223        20040407
     EP 1610785           B1    20070822
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
     JP 2006522786        T     20061005    JP 2006-506245        20040407
     AT 370733            T     20070915    AT 2004-726223        20040407
     ES 2293245           T3    20080316    ES 2004-726223        20040407
     US 20060199841       A1    20060907    US 2005-551510        20050929
     NO 2005005254        A     20060106    NO 2005-5254          20051108
PRIORITY APPLN. INFO.:                       HU 2003-929        A  20030409
                                             WO 2004-HU32       W  20040407

L16  ANSWER 7 OF 7  CAPLUS  COPYRIGHT 2008 ACS on STN
AB   Specific binding of [3H]haloperidol (HPD) in the presence of 25 nM
     spiperone was saturable and of high affinity (Kd = 1.96 ± 1.31 nM, Bmax
     = 2.37 ± 0.27 pmol/mg protein, n = 8).  Among the 29 antipsychotics
     tested in inhibition studies, bromoperidol and HPD were the most post
     inhibitors (Ki = 0.9 nM, 1.0 nM, resp.).  The conventional antipsychotics
     moperone, timiperone etc. and the novel promising drugs YM-09151, Y-516,
     BMY-14802, and remoxipride potently inhibited [3H]HPD binding with the Ki
     in the range of low to moderate nanomolar.  On the other hand, among the
     other 27 drugs tested, the antispasmodics eperisone and tolperisone, the
     antiischemic agents ifenprodil, the Ca2+ antagonist fluranizine and
     cinnarizine, and the antitussive carbetapentanece, cloperastine, and
     dextromethorphan were especially potent inhibitors.  These results suggest that
     σ receptors may be potential sites of action for anti-ischemic as
     well as antipsychotic drugs, i.e., σ receptors mediate the
     neuroprotective effects of certain antiischemic agents by affecting the
     N-methyl-D-aspartate receptor complex.
ACCESSION NUMBER:         1991:550182  CAPLUS
DOCUMENT NUMBER:          115:150182
ORIGINAL REFERENCE NO.:   115:25498h,25499a
TITLE:                    Pharmacological specificity of antipsychotic,
                          antiischemic and some other drug for σ receptors
                          labeled with [3H]haloperidol
AUTHOR(S):                Zushi, Yoshifumi
CORPORATE SOURCE:         Med. Sch., Okayama Univ., Okayama, 700, Japan
SOURCE:                   Okayama Igakkai Zasshi (1991), 103(4), 281-92
                          CODEN: OIZAAV; ISSN: 0030-1558
DOCUMENT TYPE:            Journal
LANGUAGE:                 Japanese


=> d l16 abs hitstr ibib 1-7

L16  ANSWER 1 OF 7  CAPLUS  COPYRIGHT 2008 ACS on STN
AB   Disclosed herein is are methods to treat neuropsychiatric diseases
     including psychosis.  Treatment is carried out by administering a
```

therapeutically effective amount of N-desmethylclozapine to a patient suffering from a neuropsychiatric disease.

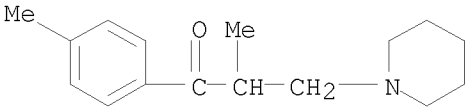
IT 125-71-3, Dextromethorphan 728-88-1, Tolperisone
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(desmethylclozapine to treat psychosis)

RN 125-71-3 CAPLUS
CN Morphinan, 3-methoxy-17-methyl-, (9α,13α,14α)- (CA INDEX NAME)

Absolute stereochemistry.



RN 728-88-1 CAPLUS
CN 1-Propanone, 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)- (CA INDEX NAME)



ACCESSION NUMBER: 2008:10517 CAPLUS
DOCUMENT NUMBER: 148:93259
TITLE: Use of n-desmethylclozapine to treat psychosis
INVENTOR(S): Weiner, David; Van Kammen, Daniel P.; Corritori, Suzana
PATENT ASSIGNEE(S): Acadia Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 88pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008002602	A1	20080103	WO 2007-US14897	20070626

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,

BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2006-817010P P 20060627

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

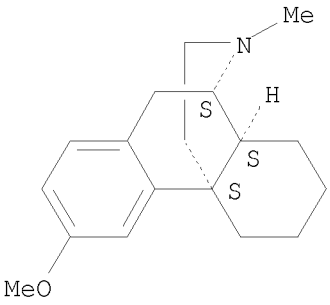
AB Cytochromes P 450 3A4, 2D6, and 2C9 metabolize a large fraction of drugs. Knowing where these enzymes will preferentially oxidize a mol., the regioselectivity, allows medicinal chemists to plan how best to block its metabolism The authors present QSAR-based regioselectivity models for these enzymes calibrated against compiled literature data of drugs and drug-like compds. These models are purely empirical and use only the structures of the substrates, in contrast to those models that simulate a specific mechanism like hydrogen radical abstraction, and/or use explicit models of active sites. The authors most predictive models use three substructure descriptors and two phys. property descriptors. Descriptor importance from the random forest QSAR method show that other factors than the immediate chemical environment and the accessibility of the hydrogen affect regioselectivity in all three isoforms. The cross-validated predictions of the models are compared to predictions from the authors earlier mechanistic model (Singh et al. J. Med. Chemical 2003, 46, 1330-1336) and predictions from MetaSite (Cruciani et al. J. Med. Chemical 2005, 48, 6970-6979).

IT 125-71-3, Dextromethorphan 728-88-1, Tolperisone
RL: PKT (Pharmacokinetics); PRP (Properties); BIOL (Biological study)
(empirical regioselectivity models for human cytochromes P 450 3A4, 2D6, and 2C9 in relation to drug metabolism)

RN 125-71-3 CAPLUS

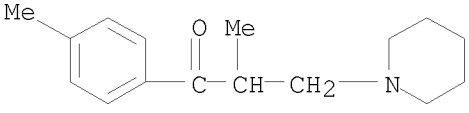
CN Morphinan, 3-methoxy-17-methyl-, (9α,13α,14α)- (CA INDEX NAME)

Absolute stereochemistry.



RN 728-88-1 CAPLUS

CN 1-Propanone, 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)- (CA INDEX NAME)



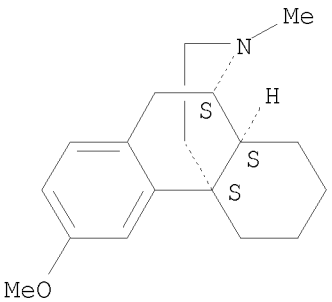
ACCESSION NUMBER: 2007:655403 CAPLUS

DOCUMENT NUMBER: 147:226154

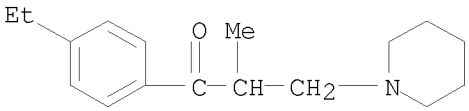
TITLE: Empirical Regioselectivity Models for Human Cytochromes P450 3A4, 2D6, and 2C9
AUTHOR(S): Sheridan, Robert P.; Korzekwa, Kenneth R.; Torres, Rhonda A.; Walker, Matthew J.
CORPORATE SOURCE: Molecular Systems Department, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(14), 3173-3184
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AB A rapid, selective and robust direct-injection LC/hybrid tandem MS method has been developed for simultaneous screening of more than 250 basic drugs in the supernatant of enzyme hydrolyzed equine urine. Analytes, trapped using a short HLB extraction column, are refocused and separated on a Sunfire C18 anal. column using a controlled differential gradient generated by proportional dilution of the first column's eluent with water. Independent data acquisition (IDA) was configured to trigger a sensitive enhanced product ion (EPI) scan when a multiple reaction monitoring (MRM) survey scan signal exceeded the defined criteria. The decision on whether or not to report a sample as a pos. result was based upon both the presence of a MRM response within the correct retention time range and a qual. match between the EPI spectrum obtained and the corresponding reference standard Ninety seven percent of the drugs targeted by this method met our detection criteria when spiked into urine at 100 ng/mL; 199 were found at 10 ng/mL, 83 at 1 ng/mL and 4 at 0.1 ng/mL.
IT 125-71-3, Dextromethorphan 64840-90-0, Eperisone
RL: ANT (Analyte); ANST (Analytical study)
(screening for basic drugs in equine urine using direct-injection differential-gradient LC-LC coupled to hybrid tandem MS/MS)
RN 125-71-3 CAPLUS
CN Morphinan, 3-methoxy-17-methyl-, (9α,13α,14α)- (CA INDEX NAME)

Absolute stereochemistry.



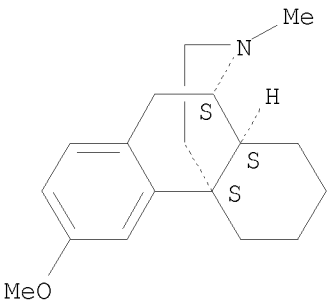
RN 64840-90-0 CAPLUS
CN 1-Propanone, 1-(4-ethylphenyl)-2-methyl-3-(1-piperidinyl)- (CA INDEX NAME)



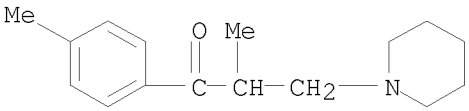
ACCESSION NUMBER: 2006:452736 CAPLUS
DOCUMENT NUMBER: 145:97622
TITLE: Screening for basic drugs in equine urine using direct-injection differential-gradient LC-LC coupled to hybrid tandem MS/MS
AUTHOR(S): Stanley, Shawn M. R.; Foo, Hsiao Ching
CORPORATE SOURCE: Singapore Race Course, The Singapore Turf Club Laboratory, Singapore, 738078, Singapore
SOURCE: Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2006), 836(1-2), 1-14
CODEN: JCBAAI; ISSN: 1570-0232
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AB Disclosed herein is a method to treat neuropsychiatric diseases including psychosis, affective disorders, dementia, neuropathic pain, and glaucoma. Treatment is carried out by administering a therapeutically effective amount of N-desmethylclozapine to a patient suffering from a neuropsychiatric disease.
IT 125-71-3, Dextromethorphan 728-88-1, Tolperisone
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(use of desmethylclozapine to treat human neuropsychiatric disease)
RN 125-71-3 CAPLUS
CN Morphinan, 3-methoxy-17-methyl-, (9α,13α,14α)- (CA INDEX NAME)

Absolute stereochemistry.



RN 728-88-1 CAPLUS
CN 1-Propanone, 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)- (CA INDEX NAME)



ACCESSION NUMBER: 2005:1200866 CAPLUS
DOCUMENT NUMBER: 143:452893
TITLE: Use of N-desmethylclozapine to treat human neuropsychiatric disease
INVENTOR(S): Weiner, David M.; Brann, Mark R.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 913,117.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

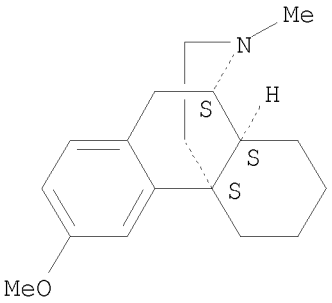
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050250767	A1	20051110	US 2005-98892	20050404
US 20040224942	A1	20041111	US 2004-761787	20040121
US 20050085463	A1	20050421	US 2004-913117	20040805
AU 2005271513	A2	20060216	AU 2005-271513	20050804
AU 2005271513	A1	20060216		
CA 2576153	A1	20060216	CA 2005-2576153	20050804
WO 2006017614	A1	20060216	WO 2005-US27645	20050804
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1778244	A1	20070502	EP 2005-802835	20050804
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 101094674	A	20071226	CN 2005-80033997	20050804
JP 2008509147	T	20080327	JP 2007-524968	20050804
US 20060194831	A1	20060831	US 2006-416565	20060503
US 20060199807	A1	20060907	US 2006-417069	20060503
US 20070275957	A1	20071129	US 2007-671405	20070205

PRIORITY APPLN. INFO.:		
US 2003-442690P	P	20030123
US 2004-761787	A2	20040121
US 2004-913117	A2	20040805
US 2004-617553P	P	20041008
US 2005-98892	A	20050404
WO 2005-US27645	W	20050804

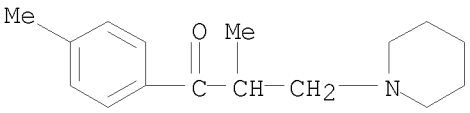
L16 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AB Disclosed herein is a method to treat neuropsychiatric diseases including psychosis, affective disorders, dementia, neuropathic pain, and glaucoma. Treatment is carried out by administering a therapeutically effective amount of N-desmethylclozapine to a patient suffering from a neuropsychiatric

disease.
IT 125-71-3, Dextromethorphan 728-88-1, Tolperisone
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(use of N-desmethylclozapine to treat human neuropsychiatric disease)
RN 125-71-3 CAPLUS
CN Morphinan, 3-methoxy-17-methyl-, (9α,13α,14α)- (CA INDEX NAME)

Absolute stereochemistry.



RN 728-88-1 CAPLUS
CN 1-Propanone, 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)- (CA INDEX NAME)



ACCESSION NUMBER: 2005:349001 CAPLUS
DOCUMENT NUMBER: 142:386016
TITLE: Use of N-desmethylclozapine to treat human neuropsychiatric disease
INVENTOR(S): Weiner, David M.; Brann, Mark R.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S Ser. No. 761,787.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

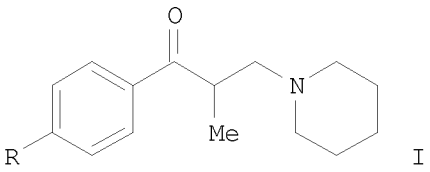
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050085463	A1	20050421	US 2004-913117	20040805
US 20040224942	A1	20041111	US 2004-761787	20040121
US 20050250767	A1	20051110	US 2005-98892	20050404
AU 2005271513	A2	20060216	AU 2005-271513	20050804
AU 2005271513	A1	20060216		
CA 2576153	A1	20060216	CA 2005-2576153	20050804
WO 2006017614	A1	20060216	WO 2005-US27645	20050804

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,

LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM

EP 1778244	A1	20070502	EP 2005-802835		20050804
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR					
CN 101094674	A	20071226	CN 2005-80033997		20050804
JP 2008509147	T	20080327	JP 2007-524968		20050804
US 20060194831	A1	20060831	US 2006-416565		20060503
US 20060199807	A1	20060907	US 2006-417069		20060503
US 20070275957	A1	20071129	US 2007-671405		20070205
IN 2007KN00526	A	20070706	IN 2007-KN526		20070213
PRIORITY APPLN. INFO.:			US 2003-442690P	P	20030123
			US 2004-761787	A2	20040121
			US 2004-913117	A2	20040805
			US 2004-617553P	P	20041008
			US 2005-98892	A	20050404
			WO 2005-US27645	W	20050804

L16 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
GI



I

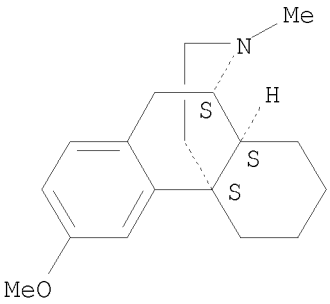
AB The present invention relates to a pharmaceutical combination for the treatment of spasticity and/or pain characterized by that the combination contains as active ingredient 70-95% weight/weight compound of formula (I), wherein R represents a Me or Et group, and 5-30 % weight/weight dextromethorphan
(chemical name: (+/-)-3-methoxy-17-methylmorphinan).

IT 125-71-3, Dextromethorphan 728-88-1 64840-90-0
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(dextromethorphan-piperidinylphenylpropanone combination for the treatment of spasticity and/or pain)

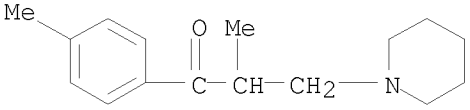
RN 125-71-3 CAPLUS

CN Morphinan, 3-methoxy-17-methyl-, (9α,13α,14α)- (CA INDEX NAME)

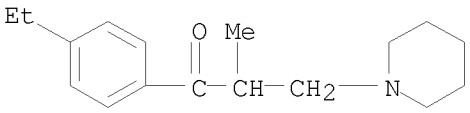
Absolute stereochemistry.



RN 728-88-1 CAPLUS
CN 1-Propanone, 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)- (CA INDEX NAME)



RN 64840-90-0 CAPLUS
CN 1-Propanone, 1-(4-ethylphenyl)-2-methyl-3-(1-piperidinyl)- (CA INDEX NAME)



ACCESSION NUMBER: 2004:872682 CAPLUS
DOCUMENT NUMBER: 141:370535
TITLE: Pharmaceutical combination for the treatment of spasticity and/or pain
INVENTOR(S): Tihanyi, Karoly; Kocsis, Pal; Nemeth, Gyoergy; Tarnawa, Istvan; Dalmadi, Balazs
PATENT ASSIGNEE(S): Richter Gedeon Vegyeszeti Gyar Rt., Hung.
SOURCE: PCT Int. Appl., 16 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089352	A2	20041021	WO 2004-HU32	20040407
WO 2004089352	A3	20041216		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,

ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

HU 2003000929	A2	20050228	HU 2003-929	20030409
HU 2003000929	A3	20050628		
EP 1610785	A2	20060104	EP 2004-726223	20040407
EP 1610785	B1	20070822		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2006522786	T	20061005	JP 2006-506245	20040407
AT 370733	T	20070915	AT 2004-726223	20040407
ES 2293245	T3	20080316	ES 2004-726223	20040407
US 20060199841	A1	20060907	US 2005-551510	20050929
NO 2005005254	A	20060106	NO 2005-5254	20051108
PRIORITY APPLN. INFO.:			HU 2003-929 A	20030409
			WO 2004-HU32 W	20040407

L16 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

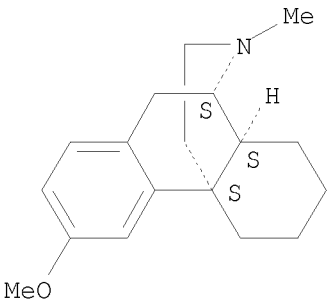
AB Specific binding of [3H]haloperidol (HPD) in the presence of 25 nM spiperone was saturable and of high affinity (Kd = 1.96 ± 1.31 nM, Bmax = 2.37 ± 0.27 pmol/mg protein, n = 8). Among the 29 antipsychotics tested in inhibition studies, bromoperidol and HPD were the most post inhibitors (Ki = 0.9 nM, 1.0 nM, resp.). The conventional antipsychotics moperone, timiperone etc. and the novel promising drugs YM-09151, Y-516, BMY-14802, and remoxipride potently inhibited [3H]HPD binding with the Ki in the range of low to moderate nanomolar. On the other hand, among the other 27 drugs tested, the antispasmodics eperisone and tolperisone, the antiischemic agents ifenprodil, the Ca2+ antagonist fluranizine and cinnarizine, and the antitussive carbetapentanece, cloperastine, and dextromethorphan were especially potent inhibitors. These results suggest that σ receptors may be potential sites of action for anti-ischemic as well as antipsychotic drugs, i.e., σ receptors mediate the neuroprotective effects of certain antiischemic agents by affecting the N-methyl-D-aspartate receptor complex.

IT 125-71-3 728-88-1, Tolperisone 64840-90-0, Eperisone
RL: BIOL (Biological study)
(brain σ-receptor binding of, pharmacol. specificity in relation to)

RN 125-71-3 CAPLUS

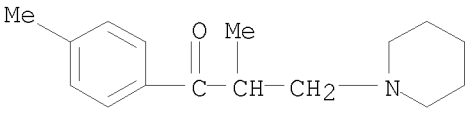
CN Morphinan, 3-methoxy-17-methyl-, (9α,13α,14α)- (CA INDEX NAME)

Absolute stereochemistry.

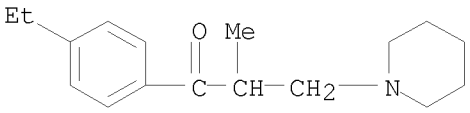


RN 728-88-1 CAPLUS

CN 1-Propanone, 2-methyl-1-(4-methylphenyl)-3-(1-piperidinyl)- (CA INDEX NAME)



RN 64840-90-0 CAPLUS
CN 1-Propanone, 1-(4-ethylphenyl)-2-methyl-3-(1-piperidinyl)- (CA INDEX NAME)



ACCESSION NUMBER: 1991:550182 CAPLUS
DOCUMENT NUMBER: 115:150182
ORIGINAL REFERENCE NO.: 115:25498h,25499a
TITLE: Pharmacological specificity of antipsychotic, antiischemic and some other drug for σ receptors labeled with [3H]haloperidol
AUTHOR(S): Zushi, Yoshifumi
CORPORATE SOURCE: Med. Sch., Okayama Univ., Okayama, 700, Japan
SOURCE: Okayama Igakkai Zasshi (1991), 103(4), 281-92
CODEN: OIZAAV; ISSN: 0030-1558
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

=> d his

(FILE 'HOME' ENTERED AT 18:45:04 ON 12 AUG 2008)

FILE 'REGISTRY' ENTERED AT 18:45:17 ON 12 AUG 2008
L1 1 S "TOLPERISONE"/CN
L2 1 S "EPERISONE"/CN
L3 2 S L1 OR L2
L4 STRUCTURE UPLOADED
L5 7 SEA SSS SAM L4

FILE 'CAPLUS' ENTERED AT 18:53:45 ON 12 AUG 2008
S L4

FILE 'REGISTRY' ENTERED AT 18:54:04 ON 12 AUG 2008
L6 7 S L4 PLU=ON

FILE 'CAPLUS' ENTERED AT 18:54:04 ON 12 AUG 2008
L7 6 S L6 PLU=ON
L8 0 S L6 AND PAIN
L9 0 S L6 AND SPASTICITY
L10 0 S L6 AND SPASM
L11 0 S L6 AND NMDA
L12 1 S (L1 OR L2) AND NMDA
L13 18 S (L1 OR L2) AND PAIN

FILE 'REGISTRY' ENTERED AT 19:03:12 ON 12 AUG 2008
L14 0 S "DEXTROMETHOPHAN"/CN

L15 1 S "DEXTROMETHORPHAN"/CN

FILE 'CAPLUS' ENTERED AT 19:03:55 ON 12 AUG 2008
L16 7 S (L1 OR L2) AND L15